10/516,292 03/28/2010

=> screen 1947 AND 1992 AND 2004 AND 1970 AND 1839

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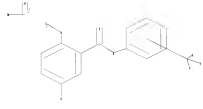

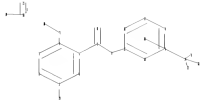

chain nodes :
7 8 9 17 18 19 20 21 24 25 26 27 29
ring nodes :
1 2 3 4 5 6 10 11 12 13 14 15

10/516,292 03/28/2010

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chain bonds :
1-29  4-17  5-7  7-8  7-9  9-11  17-18  19-20  20-21  24-25  24-26  24-27
ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  10-11  10-15  11-12  12-13  13-14  14-15
exact/norm bonds :
1-29  4-17  7-8  7-9  9-11  17-18  20-21
exact bonds :
5-7  19-20  24-25  24-26  24-27
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  10-11  10-15  11-12  12-13  13-14  14-15


G1:H,[*1]

Hydrogen count :
9:= exact 1  14:= exact 1
Match level :
1:Atom  2:Atom  3:Atom  4:Atom  5:Atom  6:Atom  7:CLASS  8:CLASS  9:CLASS  10:Atom
11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  17:CLASS  18:CLASS  19:CLASS  20:CLASS
 21:CLASS  24:CLASS
25:CLASS  26:CLASS  27:CLASS  28:Atom  29:CLASS



L2      STRUCTURE UPLOADED

=> que L2 AND L1

L3   QUE L2 AND L1

=> s l3 sss sam
SAMPLE SEARCH INITIATED 19:10:27 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -      783 TO ITERATE

100.0% PROCESSED      783 ITERATIONS                              19 ANSWERS
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        13982 TO    17338
PROJECTED ANSWERS:             119 TO      641

L4           19 SEA SSS SAM L2 AND L1

=> s l3 sss full
FULL SEARCH INITIATED 19:10:33 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -    16514 TO ITERATE

100.0% PROCESSED    16514 ITERATIONS                            407 ANSWERS
SEARCH TIME: 00.00.01

L5          407 SEA SSS FUL L2 AND L1

=> file caplus

=> s l5
L6          191 L5
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         65850 CANCERS
        464879 CANCER
                 (CANCER OR CANCERS)
        587717 NEOPLASM
         38720 NEOPLASMS
        605087 NEOPLASM
                 (NEOPLASM OR NEOPLASMS)
        720847 ?TUMOR
        537770 TUMOR
        193641 TUMORS
        596668 TUMOR
                 (TUMOR OR TUMORS)
        537770 "TUMOR"
        193641 "TUMORS"
        596668 "TUMOR"
                 ("TUMOR" OR "TUMORS")
        996713 "PLANT"
        535385 "PLANTS"
       1214068 "PLANT"
                 ("PLANT" OR "PLANTS")
          1313 "TUMOR, PLANT"
                 ("TUMOR"(W)"PLANT")
         45358 MELANOMA
          4373 MELANOMAS
            19 MELANOMATA
         45949 MELANOMA
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          8287 LEUKEMIAS
        131705 LEUKEMIA
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         25039 MYELOMA
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         49720 LYMPHOMA
         10802 LYMPHOMAS
         52011 LYMPHOMA
                 (LYMPHOMA OR LYMPHOMAS)
            55 RHABDOMYOMA
            20 RHABDOMYOMAS
            63 RHABDOMYOMA
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         59159 ?SARCOMA
         43065 ?BLASTOMA
L7      1167562 CANCER OR NEOPLASM OR ?TUMOR OR (TUMOR OR "TUMOR, PLANT") OR
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                ?SARCOMA OR ?BLASTOMA

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L8           31 L6 AND L7

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L9           11 L8 AND PY<2005
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L9 ANSWER 6 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:991336 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 140:42202
TITLE: Preparation of hydroxybenzamide, naphthalenecarboxamide, and hydroxyheterocyclecarboxamide derivatives as anticancer agents
INVENTOR(S): Muto, Susumu; Itai, Akiko
PATENT ASSIGNEE(S): Institute of Medicinal Molecular Design. Inc., Japan
SOURCE: PCT Int. Appl., 265 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103655	A1	20031218	WO 2003-JP7121	20030605 <--
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2003242108	A1	20031222	AU 2003-242108	20030605 <--
AU 2003242108	B2	20080911		
EP 1535610	A1	20050601	EP 2003-730832	20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1658856	A	20050824	CN 2003-813312	20030605
CN 100506221	C	20090701		
US 20060014811	A1	20060119	US 2005-516292	20050705
PRIORITY APPLN. INFO.:			JP 2002-168332 A	20020610
			WO 2003-JP7121 W	20030605

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 140:42202
GI

I

AB Disclosed are drugs for the prevention and/or treatment of cancer

, which contain as the active ingredient substances selected from the group consisting of compds. represented by the general formula (I), pharmacol. acceptable salts thereof, and hydrates and solvates of both [wherein A is hydrogen or acetyl; E is 2,5- or 3,5-disubstituted Ph or an optionally substituted monocyclic or fused-polycyclic heteroaryl group (exclusive of (1) fused -polycyclic heteroaryl whose benzene ring is bonded directly to the -CONH- group, (2) unsubstituted thiazol-2-yl, and (3) unsubstituted benzothiazol-2-yl); and Z is arene which may have a substituent in addition to the groups represented by the general formulas: -O-A (wherein A is as defined above) and -CONH-E (wherein E is as defined above) or heteroarene which may have a substituent in addition to the groups represented by the general formulas: -O-A (wherein A is as defined above) and -CONH-E (wherein E is as defined above)]. The compds. I including N-phenylhydroxybenzamide (N-phenylsalicylamide), N-phenylhydroxynaphthalenecarboxamide, N-heterocyclylsalicylamide, N-phenylpyridinecarboxamide, N-phenylhydroxythiophenecarboxamide, N-phenylquinoxalinecarboxamide, and N-phenylindolecarboxamide derivs. in vitro inhibited the proliferation of Jurkat, MIA PACA-2, RD, HepG2, and A549 human cancer cells.
N-[3,5-bis(trifluoromethyl)phenyl]-4-chloro-2-hydroxybenzamide in vitro inhibited the proliferation of B16 melanoma, HT-1080 fibrosarcoma, NB-1 neuroblastoma, and HMC-1-8 breast cancer cells and in vivo metastasis of B16 melanoma in mice.

L9 ANSWER 7 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2003:991335 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 140:42201
TITLE: Preparation of hydroxybenzamide, naphthalenecarboxamide, and hydroxyheterocyclecarboxamide derivatives as transcription factor NF-κB activation inhibitors
INVENTOR(S): Muto, Susumu; Itai, Akiko
PATENT ASSIGNEE(S): Institute of Medicinal Molecular Design. Inc., Japan
SOURCE: PCT Int. Appl., 286 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003103654	A1	20031218	WO 2003-JP7119	20030605 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
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AU 2003242098	A1	20031222	AU 2003-242098	20030605 <--
AU 2003242098	B2	20081120		
EP 1535609	A1	20050601	EP 2003-730830	20030605
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,				

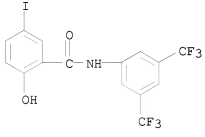
IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
CN 1658857 A 20050824 CN 2003-813313 20030605
CN 100464742 C 20090304
US 20060089395 A1 20060427 US 2005-516294 20050912
US 20080311074 A1 20081218 US 2008-81162 20080411
PRIORITY APPLN. INFO.: JP 2002-168924 A 20020610
WO 2003-JP7119 W 20030605
US 2005-516294 A3 20050912
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 140:42201
GI

I

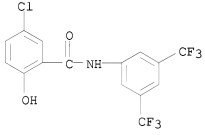
AB Disclosed are drugs having an inhibitory activity against transcription factor NF-κB activation, which contain as the active ingredient substances selected from the group consisting of compds. represented by the general formula (I), pharmacol. acceptable salts thereof, and hydrates and solvates of both [wherein A is hydrogen or acetyl; E is 2,5- or 3,5-disubstituted Ph or an optionally substituted monocyclic or fused-polycyclic heteroaryl group (exclusive of (1) fused -polycyclic heteroaryl whose benzene ring is bonded directly to the -CONH- group, (2) unsubstituted thiazol-2-yl, and (3) unsubstituted benzothiazol-2-yl); and Z is arene which may have a substituent in addition to the groups represented by the general formulas: -O-A (wherein A is as defined above) and -CONH-E (wherein E is as defined above) or heteroarene which may have a substituent in addition to the groups represented by the general formulas: -O-A (wherein A is as defined above) and -CONH-E (wherein E is as defined above)]. Also disclosed are (1) inhibitors against production and release of inflammatory mediators and immunosuppressants and (2) drugs for prevention and/or treatment of chronic articular rheumatism. The compds. I including N-phenylhydroxybenzamide (N-phenylsalicylamide), N-phenylhydroxynaphthalenecarboxamide, N-heterocyclylsalicylamide, N-phenylpyridinecarboxamide, N-phenylhydroxythiophenecarboxamide, N-phenylquinoxalinecarboxamide, and N-phenylindolecarboxamide derivs. exhibited the inhibition of (1) TNF-α-stimulated activation of NF-κB (2) TNF-α-stimulated production of IL-6, IL-8, and PGE2 in human synoviocyte (RA-pos.) cells, (3) collagen-induced inflammation in mice, (4) myocardial ischemic reperfusion disorder in rats, and (5) proliferation of smooth muscle cells of normal coronary artery blood vessel. Some com. available compds. were selected as NF-κB inhibitors (ligands) by virtual screening using a three-dimensional database automated retrieval software based on a protein structure of NF-κB. The activity of the selected compds. were confirmed by reporter assay for inhibition of TNF-α-stimulated activation of NF-κB and an assay for inhibition of NF-α-stimulated production of inflammatory mediators.
IT 906-38-7P 978-62-1P 982-71-8P

439144-26-0P 439144-29-3P 439144-43-1P
439144-46-4P 439144-53-3P 439144-65-7P
439144-78-2P 634185-07-2P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of hydroxybenzamide, naphthalenecarboxamide, and hydroxyheterocyclecarboxamide derivs. as transcription factor NF-κB activation inhibitors)

RN 906-38-7 CAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-2-hydroxy-5-iodo- (CA INDEX NAME)



RN 978-62-1 CAPLUS
CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-5-chloro-2-hydroxy- (CA INDEX NAME)



L9 ANSWER 8 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:754333 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 137:279214
TITLE: Preparation of benzoic acid derivatives as nuclear factor κB inhibitors
INVENTOR(S): Suzuki, Kenji; Nunokawa, Youichi; Ogou, Naohisa
PATENT ASSIGNEE(S): Suntory Limited, Japan; Suntory Biomedical Research Limited
SOURCE: PCT Int. Appl., 243 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002076918	A1	20021003	WO 2002-JP3017	20020327 <--
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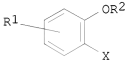
RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR				
CA 2410816	A1	20021003	CA 2002-2410816	20020327 <--
BR 2002004678	A	20030429	BR 2002-4678	20020327 <--
EP 1314712	A1	20030528	EP 2002-708696	20020327 <--
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI, CY, TR				
HU 2003002479	A2	20031128	HU 2003-2479	20020327 <--
US 20040122244	A1	20040624	US 2002-296810	20021127 <--
US 7064124	B2	20060620		
PRIORITY APPLN. INFO.:			JP 2001-91003 A	20010327
			WO 2002-JP3017 W	20020327

ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 137:279214
GI



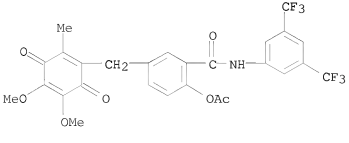
I

AB The title compds. I [R1 = (1,4-benzoquinon-2-yl)methyl (with substituents selected from H, alkyl, etc.) (generic structure given), etc.; R2 = H, (un)substituted alkyl, etc.; X = carboxyl (which may esterified or amidated)] are prepared In an in vitro test for nuclear factor κB inhibiting activity, N-[5-(5,6-dimethoxy-3-methyl-1,4-benzoquinon-2-yl)methyl-2-hydroxybenzoyl]-4-aminobenzoic acid Et ester showed IC50 value of 3 μg/mL.

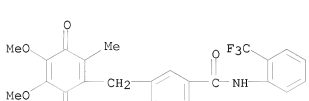
IT 464214-65-1P 464215-03-0P 464215-09-6P
RL: PAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation of benzoic acid derivs. as nuclear factor κB inhibitors)

RN 464214-65-1 CAPLUS

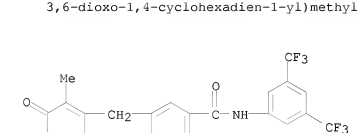
CN Benzamide, 2-(acetyloxy)-N-[3,5-bis(trifluoromethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]- (CA INDEX NAME)



RN 464215-03-0 CAPLUS
CN Benzamide, 2-(acetyloxy)-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-N-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)



CN Benzamide, N-[3,5-bis(trifluoromethyl)phenyl]-5-[(4,5-dimethoxy-2-methyl-3,6-dioxo-1,4-cyclohexadien-1-yl)methyl]-2-hydroxy- (CA INDEX NAME)



RN 464215-04-1 CAPLUS

L9 ANSWER 9 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 2002:487387 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 137:63257
TITLE: Preparation of benzamides as inhibitors of production and release of inflammatory cytokines
INVENTOR(S): Muto, Susumu; Nagano, Tatsuo; Saotome, Tomomi; Itai, Akiko
PATENT ASSIGNEE(S): Institute of Medicinal Molecular Design Inc., Japan
SOURCE: PCT Int. Appl., 313 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002049632	A1	20020627	WO 2001-JP11084	20011218 <--
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RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH,				

CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR,
BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

CA 2431083	A1	20020627	CA 2001-2431083	20011218	<--
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EP 1844766	A2	20071017	EP 2007-15076	20011218	
EP 1844766	A3	20090429			
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EP 1847263	A2	20071024	EP 2007-15427	20011218	
EP 1847263	A3	20090826			
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JP 4224566	B2	20090218	JP 2002-550974	20011218	
KR 2009090406	A	20090825	KR 2009-716971	20011218	
US 20040259877	A1	20041223	US 2004-433619	20040219	<--
HK 1063433	A1	20080905	HK 2004-106223	20040819	
US 20080249071	A1	20081009	US 2007-835997	20070808	
US 20090192122	A2	20090730			
US 20080318956	A1	20081225	US 2007-835978	20070808	
PRIORITY APPLN. INFO.:			JP 2000-383202	A 20001218	
			CN 2001-822716	A3 20011218	
			EP 2001-271124	A3 20011218	
			WO 2001-JP11084	W 20011218	
			KR 2003-708036	A3 20030616	
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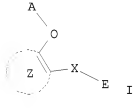
ASSIGNMENT HISTORY FOR US PATENT AVAILABLE IN LSUS DISPLAY FORMAT
OTHER SOURCE(S): MARPAT 137:63257
GI



I

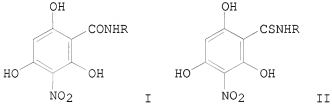
AB The title compds. I (wherein X is a connecting group; A is hydrogen or acetyl; E is aryl or heteroaryl; and Z is arene or heteroarene) are prepared In an in vitro test using cells, 5-chloro-2-hydroxy-N-(4-methoxynaphthalen-2-yl)benzamide at 1 μg/mL gave 95.1% inhibition of NF-κB activation.

L9 ANSWER 10 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1992:143846 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 116:143846
ORIGINAL REFERENCE NO.: 116:24085a,24088a
TITLE: Tumor promoter inhibitors containing nitrophloroglucinol derivatives

INVENTOR(S): Honda, Ichiro; Tokuda, Harukuni; Nishino, Hoyoku; Yoshida, Shigeo; Kozuka, Mutsuo; Yoneyama, Koichi
PATENT ASSIGNEE(S): Japan Tobacco, Inc., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

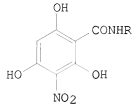
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03271222	A	19911203	JP 1990-69852	19900322 <--

PRIORITY APPLN. INFO.: JP 1990-69852 19900322
OTHER SOURCE(S): MARPAT 116:143846
GI



AB Antitumor agents which inhibit tumor promoters contain nitrophloroglucinol derivs. I [R = C1-18 straight-chain alkyl, cyclohexyl, substituted Ph, phenylalkyl (containing C1-4 alkyl)] or II (R = C1-10 straight-chain alkyl). I (R = Me) at 100-fold dilution inhibited 12-O-tetradecanoylphorbol-13-acetate (III)-induced production of Epstein-Barr virus early antigens by 92.35%. Topical application of I to mice inhibited tumors induced by DMBA and III.

L9 ANSWER 11 OF 11 CAPLUS COPYRIGHT 2010 ACS on STN
ACCESSION NUMBER: 1991:597735 CAPLUS <<LOGINID::20100328>>
DOCUMENT NUMBER: 115:197735
ORIGINAL REFERENCE NO.: 115:33489a,33492a
TITLE: Inhibitory effects of 3-nitro-2,4,6-trihydroxybenzamides on Epstein-Barr virus early antigen induction
AUTHOR(S): Honda, Ichiro; Tokuda, H.; Kozuka, M.; Yoneyama, K.; Nishino, H.; Iwashima, A.; Shibagaki, M.; Noma, M.; Takahashi, N.; Yoshida, S.
CORPORATE SOURCE: Life Sci. Res. Lab., Japan Tob. Inc., Yokohama, 227, Japan
SOURCE: Cancer Letters (Shannon, Ireland) (1991), 59(2), 83-8
CODEN: CALEDQ; ISSN: 0304-3835
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB Inhibitory effects of a series of 3-nitro-2,4,6-trihydroxybenzamides (I; R = alkyl, benzyl, substituted Ph, etc.) of Epstein-Barr virus early antigen (EBV-EA) induction were examined using Raji cells. Some of the tested compds. showed highly inhibitory activity, the N-octyl amide derivative being the most active among them. These results suggest the possibility that 3-nitro-2,4,6-trihydroxybenzamides might be listed as novel inhibitors of tumor promotion.

IT 129235-56-9 129235-57-0
RL: BIOL (Biological study)
(Epstein-Barr virus early antigen induction inhibition by, structure in relation to)

RN 129235-56-9 CAPLUS

CN Benzamide, 2,4,6-trihydroxy-3-nitro-N-[2-(trifluoromethyl)phenyl]- (CA INDEX NAME)